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Bis(1-{[3-(cyclohexylammonio)propyl]-iminomethyl}naphthalen-2-olato)cobalt(II) dichloride dihydrate

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The Co atom in the title mononuclear cobalt(II) complex, $[Co(C_{20}H_{26}N_2O)_2]Cl_2\cdot 2H_2O$, lying on an inversion centre, is four-coordinated in a square-planar geometry by two phenolate O atoms and two imine N atoms from two Schiff base ligands.

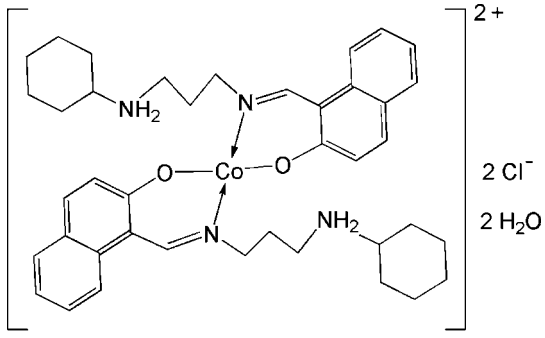
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.050
wR factor = 0.162
Data-to-parameter ratio = 19.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The ability of certain cobalt(II) complexes to bind dioxygen reversibly was discovered decades ago. Many cobalt(II) dioxygen carriers have been discovered (Rybak-Akimova *et al.*, 1997), most of them having properties which make them good candidates for industrial and/or medicinal applications. Here we report the structure of the new cobalt(II) title complex, (I).



(I)

The Co^{II} ion in (I), lying on an inversion centre, is four-coordinated by two phenolate O and two imine N atoms from two Schiff base ligands, forming a square-planar geometry, as shown in Fig. 1. All bond lengths and angles subtended at the Co centre (Table 1) are comparable with those observed in other similar cobalt(II) complexes (Qiu *et al.*, 2006; Iyere *et al.*, 2004; Chen, 2006; Zhang *et al.*, 2006).

The Cl^- counterions are linked to the solvent water molecules through intermolecular O—H···Cl hydrogen bonds (Table 2). The Cl^- counterions and the solvent water molecules are further linked to the complex molecules through intermolecular O—H···N and N—H···Cl hydrogen bonds (Table 2), forming layers parallel to the *bc* plane (Fig. 2).

Experimental

2-Hydroxy-1-naphthaldehyde (1.0 mmol, 86.3 mg), *N*-cyclohexylpropane-1,3-diamine (1.0 mmol, 156.2 mg) and $CoCl_2\cdot 6H_2O$ (0.5 mmol, 118.9 mg) were dissolved in an EtOH–H_2O solution (100 ml, 5:1 *v*/*v*). The mixture was stirred for 30 min at room temperature to give a brown solution. X-ray diffraction quality

crystals of (I) were formed after several days by slow evaporation of the solvents in air.

Crystal data

$[Co(C_{20}H_{26}N_2O)_2]Cl_2\cdot 2H_2O$
$M_r = 786.72$
Monoclinic, $P2_1/c$
$a = 11.171$ (1) Å
$b = 7.423$ (1) Å
$c = 23.654$ (3) Å
$\beta = 92.521$ (1)°
$V = 1959.6$ (4) Å^3
$Z = 2$
$D_x = 1.333$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.62$ mm^{-1}
$T = 298$ (2) K
Block, red
0.32 × 0.28 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.826$, $T_{max} = 0.851$
16510 measured reflections
4659 independent reflections
3581 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 28.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.162$
$S = 1.04$
4659 reflections
238 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0987P)^2 + 0.3207P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.70$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.826 (2)	Co1—N1	1.911 (2)
O1^{i}—Co1—O1	180.0	O1—Co1—N1	91.74 (8)
O1^{i}—Co1—N1	88.26 (8)	N1—Co1—N1^{i}	180.0

Symmetry code: (i) $-x+2, -y+2, -z+2$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2D···Cl1	0.87 (3)	2.31 (3)	3.178 (5)	179 (3)
O2—H2C···N2	0.87 (3)	2.59 (3)	3.241 (5)	133 (4)
O2—H2C···Cl1^{ii}	0.87 (3)	2.58 (2)	3.350 (6)	149 (4)
N2—H2B···Cl1^{iii}	0.90	2.24	3.133 (2)	172
N2—H2A···Cl1^{ii}	0.90	2.31	3.204 (2)	171

Symmetry codes: (ii) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x, y+1, z$.

H atoms attached to the solvent water molecule were located in a difference Fourier map and refined isotropically, with O—H distances restrained to 0.84 (1) Å, H···H distances restrained to 1.37 (2) Å, and U_{iso}(H) = 0.08 Å^2. H atoms attached to C and N atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and N—H = 0.90 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

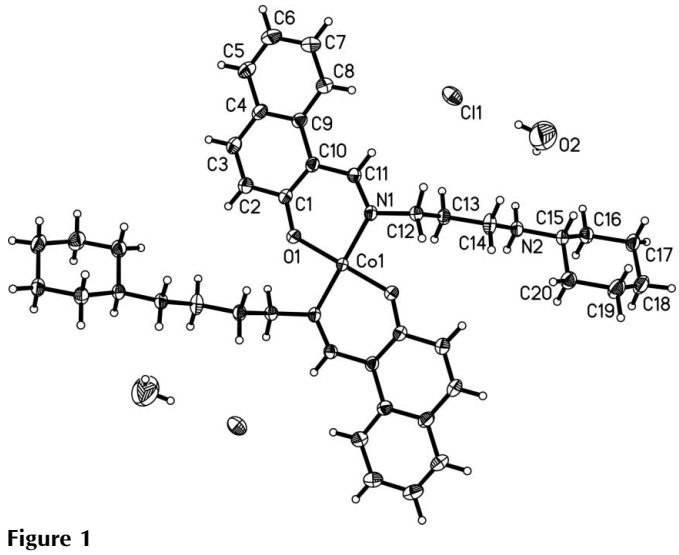


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are generated by the symmetry operator $(2-x, 2-y, 2-z)$.

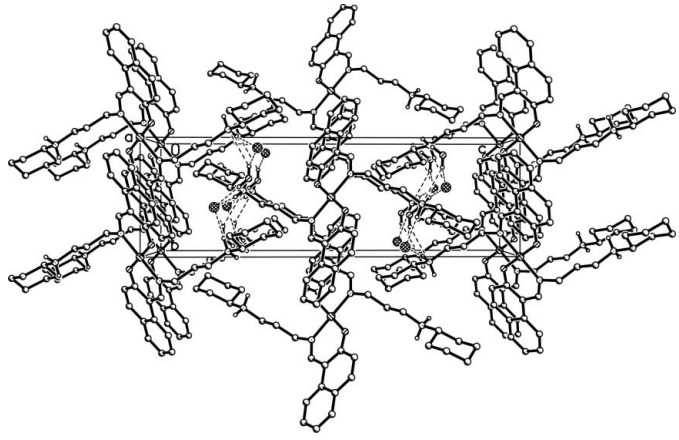


Figure 2
The crystal packing of (I). H atoms not involved in hydrogen bonds have been omitted for clarity. Hydrogen bonds are shown as dashed lines.

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